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Interface traction stress of 3D dislocation loop in anisotropic bimaterial

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ABSTRACT

By applying discrete Fast Fourier Transformation (FFT), semi-analytical solutions are developed to calculate the interface elastic fields of anisotropic bimaterial systems with perfect bonding, dislocation-like, force-like and linear spring-like interface models. Interface elastic fields are the linear superimposition of bulk stress, free surface relaxation image stress and interface traction stress (ITS) fields. Interface image energy of perfect bonding bimaterials can be solved through area integral over the interface plane, including the contribution of several componential stress fields. Calculation examples on dislocation loops within Cu–Nb bimaterial are performed to demonstrate the efficiency of such approaches. Effects of $\boldsymbol{K}^{\boldsymbol{u}}=[k_{ij}^{u}]$ for the dislocation-like, $\boldsymbol{K}^{\boldsymbol{t}}=[k_{ij}^{t}]$ for the force-like and $\boldsymbol{K}^{s}=\mathrm{diag}[\boldsymbol{K}_T, \boldsymbol{K}_N]$ for the linear spring-like imperfect interface models are investigated. Differences between perfect bonding and imperfect interface models, isotropic and anisotropic models are also studied. It is found that interface conditions and anisotropy have drastic effects on the interface elastic fields.

1. Introduction

In recent decades, bimaterial, multilayers/coatings composed of alternating layers of different materials are widely used in micro-electronics, opto-electronics, laser mirrors, and have been developed for more demanding structural applications (e.g. aircraft, rocket engines, transportation, advanced energy, nuclear reactors, etc.) (Ghoniem and Han, 2005). Stress fields that arise due to the presence of elastic modulus mismatch and crystallographic misorientation across the interface of multilayer materials are critical to understand the interaction nature between dislocations and interfaces, which can result in blocking, transmission, or absorption of the dislocation at the interfaces. When a glide dislocation approaches the interface with relatively low strength, its stress field locally shears the weak interface, and the interfacial shearing is accommodated by the nucleation and growth of interfacial dislocations, which have an attractive interaction with the incoming dislocation (Wang and Misra, 2011; Chu et al., 2013). Interface image stress will arise due to the elastic modulus mismatch across bimaterial interface planes, which appear to be the dominant source of resistance to dislocation motion from one layer to another. For a dislocation in one layer, the interface image stress is determined mainly by the elastic modulus and thicknesses of neighboring layers (Han and Ghoniem, 2005).

Analytical solution is difficult and rare for studying the elastic interaction between 3D dislocations and interfaces (Han

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et al., 2013). Point-force Green's function can be employed to derive the elastic field produced by a dislocation loop in the corresponding materials by integration over the dislocation surface (Mura, 1968; Han et al., 2013). This method is general, no matter if the dislocation is in a homogeneous or inhomogeneous, isotropic or anisotropic biomaterial, provided the corresponding point-force Green's function is known (Han et al., 2013; Han and Ghoniem, 2005; Ghoniem and Han, 2005). In an infinite homogeneous medium, using the spatial symmetry property of the Green's function, the surface integral can be reduced to a line-integral for the field induced by a dislocation loop (Han et al., 2013; Han and Pan, 2013; Mura, 1987; Hirth and Lothe, 1982). In an inhomogeneous medium, however, there is no such spatial symmetry in the Green's function, and thus no line-integral solution is available for a dislocation loop (Han et al., 2013).

The Green's functions of a point force applied in a bimaterial isotropic solid were solved by Rongved (1955) and Dundurs and Hetenyi (1965). Using Green's function for a point source in an isotropic bimaterial medium, the stress field of prismatic and glide loops was derived by integration over the area of the loop, lying in a plane parallel to the interface in a bimaterial composed of two isotropic half-spaces (Salamon and Dundurs, 1971, 1977; Dundurs and Salamon, 1972). Yu and Sanday (1991) presented a method for obtaining the elastic solution of an infinitesimal dislocation loop in an isotropic bimaterial, perfectly bonded or in frictionless contact at the interface plane. Gosling and Willis (1994) derived a line-integral expression for the stress field associated with an arbitrary dislocation in an isotropic half-space. Akarapu and Zbib (2009) constructed line-integral expressions for the displacement and stress fields induced by an arbitrarily shaped dislocation in an isotropic bimaterial. Tan and Sun (2006, 2011) obtained line-integral solutions for the stress fields induced by dislocation loops in an isotropic thin film-substrate system and multilayered heterogeneous thin-film system.

A theorem based on anisotropic Stroh's formula for calculating the image stress of infinite straight dislocations in anisotropic bicrystals has been developed by Barnett and Lothe (1974). Explicit expressions for the anisotropic Green's functions were derived by Ting and Lee (1997) in terms of the Stroh eigenvalues (Stroh, 1958; Stroh, 1962). The anisotropic half-space Green's functions were obtained by Walker (1993), and the anisotropic Green's functions of a point source in bimaterial mediums were obtained by Pan and Yuan (2000). Pan and Yang (2003) also made a brief review on the 3D Green's functions in anisotropic half-spaces. Wang and Wu (2005) obtained Green's function for an elastically anisotropic dissimilar film-substrate embedded with a screw dislocation in series form by the method of continuously distributed image dislocations. An approximate line-integral expression for the elastic field produced by dislocations in multilayered materials of elastic anisotropy was proposed by Ghoniem and Han (2005). Using anisotropic Green's function for a point source in multilayered mediums (Yang and Pan, 2002), Han and Ghoniem (2005) numerically studied the stress fields of an infinitesimal dislocation loop and finite dislocation loop within multilayers and investigated their interactions with interfaces. Line-integral expressions for the displacement and stress fields due to a 3D dislocation loop in an anisotropic elastic bimaterial (Chu et al., 2012), in a piezoelectric bimaterials (Han and Pan, 2012) and in anisotropic magneto–electro-elastic bimaterials were derived recently (Han et al., 2013). Based on the single dislocation Green's function, analytical solutions of the elastic fields due to dislocation arrays in an anisotropic bimaterial system are derived by virtue of the Cottrell summation formula (Chu and Pan, 2014). Weinberger et al. (2009) and Wu et al. (2012) developed the semi-analytical solutions for calculating image stress of approaching dislocations and dislocation loops within anisotropic half-spaces and free standing thin films.

Most of the existing results in this field dealt with classical perfect bonding model, in which the assumption that tractions and displacement are continuous across the material interface is used. However, the perfect bonding condition is a convenient idealization of more complicated phenomena. In reality, this condition is inadequate for the accurate representation of many practical cases in which interface damage (e.g. debonding, sliding and/or cracking across an interface) is focused, since it is well-known that imperfect bondings along a material interface can significantly influence its mechanical and thermal properties (Sudak and Wang, 2006). Pan (2003) obtained the 3D point-force Green's function in an anisotropic elastic bimaterial with imperfect interface conditions, where the interface displacements and traction vectors are uncoupled, and four types of interface models were studied: the classical perfect bonding model, the frictionless imperfect interface model, the dislocation-like imperfect interface model (Yu, 1998), and the force-like imperfect interface model which is similar to the dislocation-like model except that there is a jump in the tractions instead of the displacements. Besides these four models, another widely accepted model called linear spring-like model is also employed for describing the imperfect interface condition of bimaterial systems. In the linear spring-like model, the displacements and tractions are coupled: the tractions are continuous but the displacements at either side of the interface layer become discontinuous, and the jump in displacement is linearly proportional to the interfacial traction (Lene and Leguillon, 1982; Benveniste and Aboudi, 1984; Achenbach and Zhu, 1989; Hashin, 1990, 1991; Jasuik et al., 1992; Qu, 1993).

In order to understand the deformation mechanisms of materials at the nano- and micro-scales, dislocation dynamics (DD) methods have been developed to describe the plasticity of material system on the basis of direct numerical simulations of the motion, multiplication, interactions and dynamic evolution of dislocation networks in response to external loading. When performing dislocation dymamics study of materials, the exact positions and velocities of all dislocation segments at each instant should be calculated out. However, the majority of these DD approaches treat bulk isotropic materials, efficient solutions for the elastic field of 3D dislocations near free surfaces or interfaces are very few, and are not directly suitable for inclusion in the DD framework. Moreover, these approaches have limitations, either because they are restricted to the simple case of a planar free surface, treat only isotropic materials, or that they lack sufficient numerical resolution near interfaces and surfaces. The elastic field of dislocation loops of general geometry in anisotropic multilayer materials can be determined through a surface integral over the dislocation loop, provided that Green's functions are available for the specific geometry. However, surface integral forms cannot be readily incorporated into DD formulations, which are all based on line